Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 3.69e-11 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 2.95e-01

Confidence level: 6.18e-01

Nearest Neighbors from the Training Set

Image not found
Indole
Measured: 1.54e-10
Predicted: 4.80e-11

Image not found
Quinoline
Measured: 1.16e-11
Predicted: 5.13e-11

Image not found
2-Methylfuran
Measured: 6.19e-11
Predicted: 4.03e-11

Image not found
N-Methylacetamide
Measured: 5.20e-12
Predicted: 3.62e-12

Image not found
Aniline
Measured: 1.11e-10
Predicted: 3.34e-11